Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:54 am BST

PDB ID	:	4GNX
Title	:	Structure of U. maydis Replication protein A bound to ssDNA
Authors	:	Pavletich, N.P.; Fan, J.
Deposited on	:	2012-08-17
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

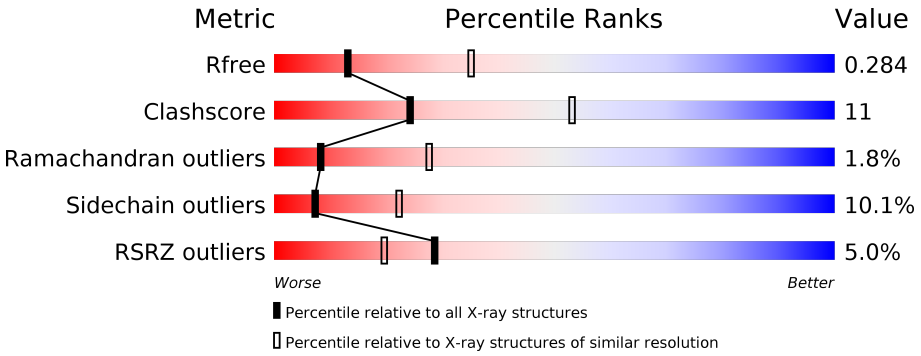
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	114	3% 64% 24% 6% • 5%
1	X	114	4% 63% 21% 9% • 5%
2	B	136	% 68% 18% • • 10%
2	Y	136	2% 64% 21% • 10%
3	C	444	5% 74% 21% • •
3	Z	444	6% 73% 22% • •

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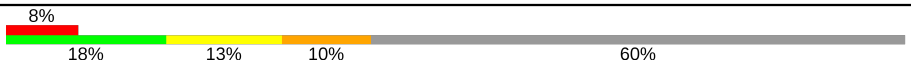
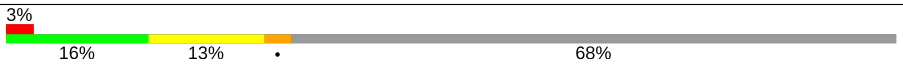
Mol	Chain	Length	Quality of chain
4	K	62	
4	L	62	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11350 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			809	505	132	168	4			
1	X	108	Total	C	N	O	S	0	0	0
			809	505	132	168	4			

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	0	0	0
			978	609	186	181	2			
2	Y	122	Total	C	N	O	S	0	0	0
			978	609	186	181	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	VAL	ALA	CONFLICT	UNP Q4PBD4
Y	173	VAL	ALA	CONFLICT	UNP Q4PBD4

- Molecule 3 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	433	Total	C	N	O	S	0	0	0
			3437	2144	600	675	18			
3	Z	433	Total	C	N	O	S	0	0	0
			3437	2144	600	675	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	314	GLN	THR	CONFLICT	UNP Q4P407
Z	314	GLN	THR	CONFLICT	UNP Q4P407

- Molecule 4 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	25	Total	C	N	O	P	0	0	0
			500	250	50	175	25			
4	L	20	Total	C	N	O	P	0	0	0
			400	200	40	140	20			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

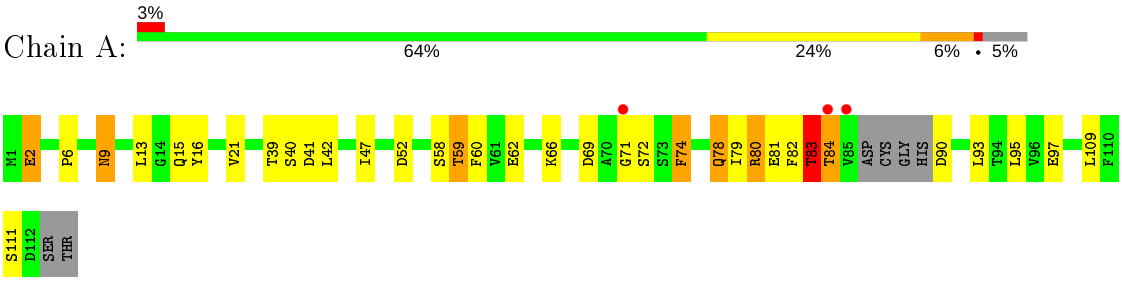
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Z	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

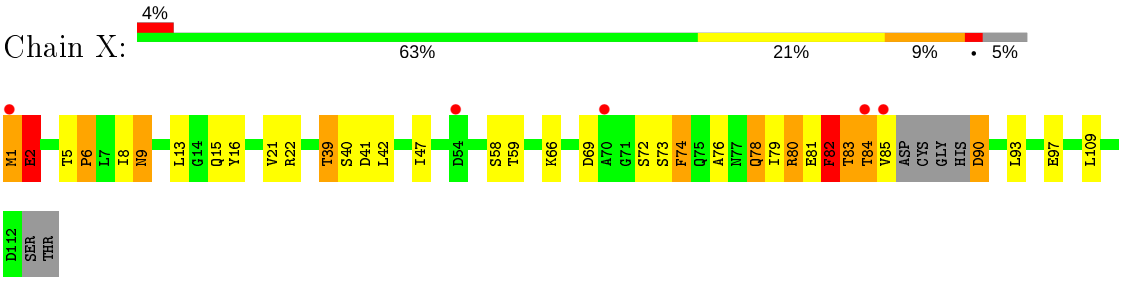
- Molecule 1: Putative uncharacterized protein

Chain A:



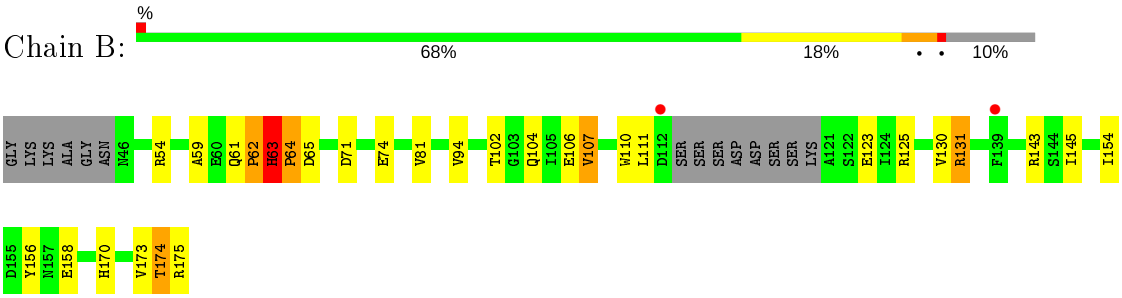
- Molecule 1: Putative uncharacterized protein

Chain X:



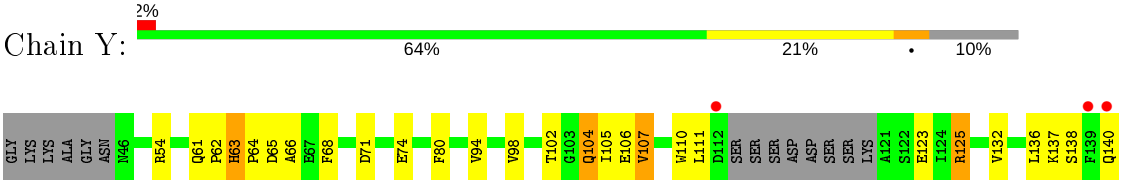
- Molecule 2: Putative uncharacterized protein

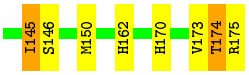
Chain B:



- Molecule 2: Putative uncharacterized protein

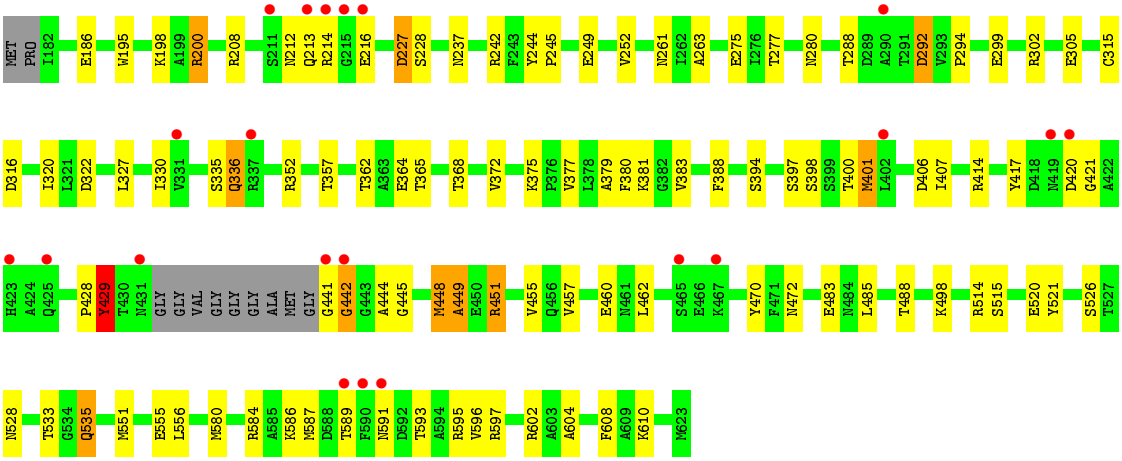
Chain Y:





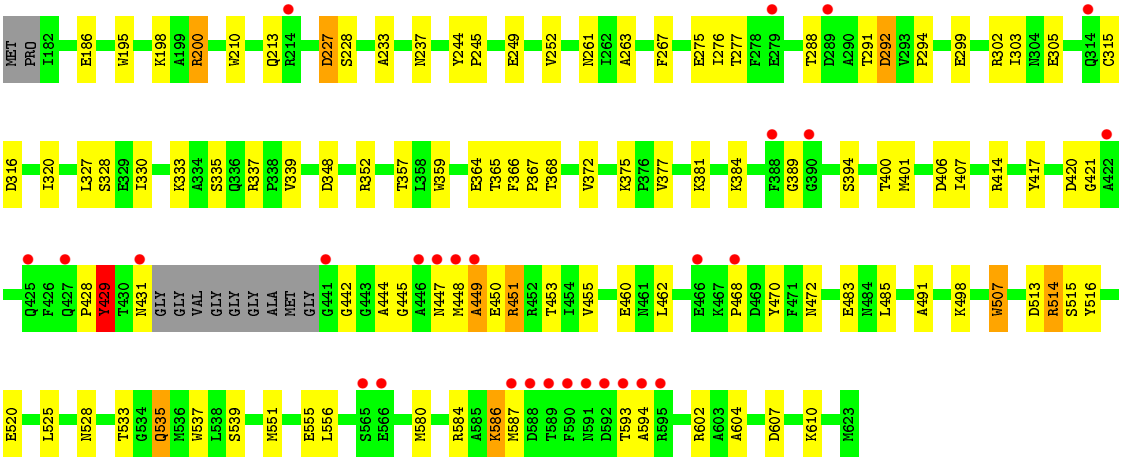
• Molecule 3: Putative uncharacterized protein

Chain C:



• Molecule 3: Putative uncharacterized protein

Chain Z:



• Molecule 4: DNA (25-MER)

Chain K:

• Molecule 4: DNA (25-MER)

Chain L:


T1 T2 T3 T4 T5 T6 T7 T8 T9 DT DT T12 T13 T14 T19 T20 T21 T22 DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.10Å 91.40Å 114.60Å 90.00° 97.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 34.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.3 (20.00-2.80) 88.1 (34.97-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.219 , 0.278 0.223 , 0.284	Depositor DCC
R_{free} test set	1498 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11350	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7967e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.59	0/818	0.77	0/1111
1	X	0.57	0/818	0.73	1/1111 (0.1%)
2	B	0.63	1/994 (0.1%)	0.72	0/1348
2	Y	0.58	1/994 (0.1%)	0.70	0/1348
3	C	0.52	1/3502 (0.0%)	0.65	1/4732 (0.0%)
3	Z	0.53	5/3502 (0.1%)	0.66	1/4732 (0.0%)
4	K	0.34	0/549	1.05	9/846 (1.1%)
4	L	0.32	0/438	0.94	3/672 (0.4%)
All	All	0.53	8/11615 (0.1%)	0.72	15/15900 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	110	TRP	CD2-CE2	5.61	1.48	1.41
2	Y	110	TRP	CD2-CE2	5.54	1.48	1.41
3	C	195	TRP	CD2-CE2	5.38	1.47	1.41
3	Z	359	TRP	CD2-CE2	5.31	1.47	1.41
3	Z	210	TRP	CD2-CE2	5.26	1.47	1.41
3	Z	507	TRP	CD2-CE2	5.25	1.47	1.41
3	Z	195	TRP	CD2-CE2	5.05	1.47	1.41
3	Z	537	TRP	CD2-CE2	5.04	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	442	GLY	N-CA-C	9.29	136.31	113.10
4	K	11	DT	P-O3'-C3'	8.87	130.34	119.70
4	L	14	DT	P-O3'-C3'	8.24	129.59	119.70
3	C	442	GLY	N-CA-C	7.94	132.95	113.10
4	K	18	DT	P-O3'-C3'	7.06	128.17	119.70
4	K	4	DT	P-O3'-C3'	6.94	128.03	119.70
4	K	10	DT	P-O3'-C3'	6.89	127.97	119.70
4	K	12	DT	P-O3'-C3'	6.41	127.39	119.70
4	K	5	DT	P-O3'-C3'	6.41	127.39	119.70
4	K	24	DT	P-O3'-C3'	5.83	126.70	119.70
4	K	8	DT	P-O3'-C3'	5.58	126.40	119.70
4	L	21	DT	P-O3'-C3'	5.25	126.00	119.70
4	L	19	DT	P-O3'-C3'	5.20	125.94	119.70
1	X	109	LEU	CA-CB-CG	5.19	127.24	115.30
4	K	17	DT	P-O3'-C3'	5.04	125.74	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	441	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	809	0	807	36	0
1	X	809	0	807	33	0
2	B	978	0	970	16	0
2	Y	978	0	970	19	0
3	C	3437	0	3315	67	0
3	Z	3437	0	3315	65	0
4	K	500	0	301	17	0
4	L	400	0	242	13	0
5	C	1	0	0	0	0
5	Z	1	0	0	0	0
All	All	11350	0	10727	242	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:63:HIS:HB3	2:Y:64:PRO:HD2	1.28	1.12
2:B:62:PRO:O	2:B:64:PRO:HD2	1.51	1.10
3:Z:451:ARG:HG3	3:Z:451:ARG:HH11	1.19	1.06
3:C:451:ARG:HG3	3:C:451:ARG:HH11	1.23	0.99
1:A:62:GLU:HB2	1:A:82:PHE:HZ	1.29	0.96
1:A:60:PHE:HD1	1:A:83:THR:HG1	1.05	0.94
1:A:83:THR:HG23	1:A:90:ASP:N	1.82	0.93
1:A:80:ARG:HA	1:A:80:ARG:HE	1.35	0.92
1:X:9:ASN:HB2	1:X:41:ASP:HB2	1.59	0.85
3:Z:498:LYS:HB2	4:L:14:DT:H5"	1.59	0.84
3:C:597:ARG:HD3	4:K:17:DT:O4	1.78	0.82
1:A:9:ASN:HB2	1:A:41:ASP:HB2	1.62	0.81
3:Z:602:ARG:HH21	3:Z:604:ALA:HB2	1.46	0.80
3:C:602:ARG:HH21	3:C:604:ALA:HB2	1.45	0.79
1:A:81:GLU:O	1:A:82:PHE:CD2	2.35	0.79
3:C:375:LYS:HG2	3:C:417:TYR:CE2	2.18	0.78
1:X:78:GLN:HA	1:X:78:GLN:HE21	1.49	0.77
3:Z:375:LYS:HG2	3:Z:417:TYR:CE2	2.19	0.77
1:A:83:THR:CG2	1:A:90:ASP:N	2.47	0.77
1:A:78:GLN:HA	1:A:78:GLN:HE21	1.48	0.76
3:Z:472:ASN:HB3	3:Z:580:MET:HE1	1.68	0.76
1:A:13:LEU:CD1	1:A:72:SER:HB2	2.15	0.76
1:X:58:SER:HB2	1:X:81:GLU:OE2	1.87	0.75
2:B:61:GLN:O	2:B:63:HIS:N	2.15	0.74
3:Z:514:ARG:NH1	3:Z:515:SER:O	2.20	0.74
3:C:551:MET:HG2	3:C:555:GLU:HB2	1.69	0.73
3:C:472:ASN:HB3	3:C:580:MET:HE1	1.69	0.73
4:K:12:DT:H2"	4:K:13:DT:OP2	1.89	0.72
3:C:514:ARG:HG2	3:C:515:SER:H	1.54	0.71
1:A:2:GLU:HA	1:A:2:GLU:OE1	1.90	0.71
3:C:397:SER:HB3	4:K:5:DT:H3	1.55	0.71
2:Y:63:HIS:HB3	2:Y:64:PRO:CD	2.14	0.70
3:Z:451:ARG:CG	3:Z:451:ARG:HH11	2.02	0.69
3:C:448:MET:O	3:C:449:ALA:CB	2.41	0.69
4:L:2:DT:H2"	4:L:3:DT:OP1	1.91	0.69
1:X:80:ARG:HA	1:X:80:ARG:HE	1.58	0.68
3:C:595:ARG:HH11	4:K:17:DT:H73	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:352:ARG:HH21	3:C:429:TYR:HA	1.59	0.67
3:C:451:ARG:HH11	3:C:451:ARG:CG	2.04	0.67
3:Z:352:ARG:HH21	3:Z:429:TYR:HA	1.60	0.66
3:C:442:GLY:O	4:K:8:DT:H5'	1.96	0.65
1:A:80:ARG:NE	1:A:80:ARG:HA	2.11	0.64
1:A:15:GLN:HE22	1:X:15:GLN:HE22	1.43	0.64
3:Z:357:THR:OG1	3:Z:444:ALA:HB3	1.97	0.64
4:K:8:DT:H2'	4:K:9:DT:C6	2.33	0.64
2:Y:63:HIS:CB	2:Y:64:PRO:HD2	2.13	0.63
1:X:13:LEU:CD1	1:X:72:SER:HB2	2.29	0.63
1:A:62:GLU:HB2	1:A:82:PHE:CZ	2.21	0.62
1:A:13:LEU:HD13	1:A:72:SER:HB2	1.81	0.62
2:B:71:ASP:OD2	2:B:170:HIS:HD2	1.81	0.62
1:X:13:LEU:HD13	1:X:72:SER:HB2	1.81	0.62
3:C:200:ARG:HB3	3:C:252:VAL:HG22	1.82	0.62
3:C:472:ASN:HB3	3:C:580:MET:CE	2.30	0.61
2:B:170:HIS:O	2:B:174:THR:HB	2.00	0.60
3:C:214:ARG:HH12	4:K:2:DT:H4'	1.66	0.60
3:Z:513:ASP:O	3:Z:514:ARG:HB2	2.00	0.60
3:Z:375:LYS:HE2	3:Z:417:TYR:OH	2.02	0.59
3:Z:447:ASN:HB2	3:Z:450:GLU:OE2	2.02	0.59
1:A:58:SER:HB2	1:A:81:GLU:OE2	2.02	0.59
1:X:2:GLU:HG2	2:Y:104:GLN:HB2	1.84	0.59
3:Z:460:GLU:HB2	3:Z:462:LEU:HD13	1.85	0.59
1:X:2:GLU:OE1	1:X:2:GLU:HA	2.03	0.59
2:Y:107:VAL:HB	2:Y:145:ILE:HB	1.85	0.59
2:B:131:ARG:HG2	2:B:131:ARG:HH11	1.68	0.59
3:C:448:MET:O	3:C:449:ALA:HB3	2.02	0.59
3:C:397:SER:CB	4:K:5:DT:H3	2.16	0.58
3:Z:448:MET:O	3:Z:449:ALA:CB	2.50	0.58
3:Z:263:ALA:HA	3:Z:275:GLU:HG2	1.84	0.58
3:C:365:THR:O	3:C:368:THR:HB	2.04	0.58
1:X:9:ASN:HA	1:X:39:THR:HG21	1.86	0.58
3:C:551:MET:HG2	3:C:555:GLU:CB	2.34	0.58
3:Z:551:MET:HG2	3:Z:555:GLU:HB2	1.84	0.58
1:A:6:PRO:HG3	1:A:16:TYR:CE2	2.39	0.57
3:Z:365:THR:O	3:Z:368:THR:HB	2.04	0.57
2:Y:170:HIS:O	2:Y:174:THR:HB	2.05	0.56
3:Z:200:ARG:HB3	3:Z:252:VAL:HG22	1.88	0.56
1:A:21:VAL:CG2	1:A:74:PHE:HZ	2.18	0.56
3:C:292:ASP:N	3:C:292:ASP:OD1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:VAL:HB	2:B:145:ILE:HB	1.88	0.56
3:C:460:GLU:HB2	3:C:462:LEU:HD13	1.88	0.56
3:Z:302:ARG:HB2	3:Z:305:GLU:HG3	1.88	0.55
3:C:587:MET:SD	3:C:596:VAL:HG22	2.45	0.55
3:Z:498:LYS:CB	4:L:14:DT:H5"	2.34	0.55
3:Z:267:PHE:HA	4:L:5:DT:H73	1.89	0.55
1:X:5:THR:O	1:X:5:THR:HG22	2.07	0.55
1:X:21:VAL:CG2	1:X:74:PHE:HZ	2.18	0.55
2:Y:71:ASP:OD2	2:Y:170:HIS:HD2	1.90	0.55
1:A:13:LEU:HD13	1:A:72:SER:CB	2.37	0.55
3:Z:451:ARG:NH1	3:Z:451:ARG:HG3	1.98	0.54
3:C:261:ASN:ND2	3:C:277:THR:OG1	2.41	0.54
3:C:498:LYS:HB2	4:K:14:DT:H5"	1.90	0.54
1:X:1:MET:O	1:X:2:GLU:O	2.25	0.54
3:Z:448:MET:O	3:Z:449:ALA:HB3	2.08	0.54
1:X:9:ASN:HD22	1:X:9:ASN:C	2.11	0.53
1:A:59:THR:HB	1:A:83:THR:OG1	2.08	0.53
4:K:18:DT:H4'	4:K:19:DT:OP2	2.08	0.53
3:Z:498:LYS:HB2	4:L:14:DT:C5'	2.33	0.53
1:X:41:ASP:O	1:X:42:LEU:HB2	2.09	0.53
2:Y:54:ARG:NH1	2:Y:102:THR:O	2.41	0.53
1:A:9:ASN:HA	1:A:39:THR:HG21	1.91	0.53
2:Y:62:PRO:O	2:Y:63:HIS:HB2	2.09	0.53
3:Z:394:SER:HB2	3:Z:445:GLY:HA3	1.89	0.53
3:Z:472:ASN:HB3	3:Z:580:MET:CE	2.36	0.53
3:C:263:ALA:HA	3:C:275:GLU:HG2	1.90	0.52
3:Z:267:PHE:HA	4:L:5:DT:C7	2.39	0.52
3:Z:200:ARG:NH1	3:Z:294:PRO:O	2.42	0.52
1:A:13:LEU:CD1	1:A:72:SER:CB	2.87	0.52
3:C:302:ARG:HB2	3:C:305:GLU:HG3	1.90	0.52
3:Z:261:ASN:ND2	3:Z:277:THR:OG1	2.42	0.52
2:Y:61:GLN:HE21	2:Y:66:ALA:H	1.58	0.52
3:C:595:ARG:NH1	4:K:17:DT:H73	2.26	0.51
2:Y:105:ILE:HD13	2:Y:145:ILE:HD13	1.92	0.51
1:A:81:GLU:O	1:A:82:PHE:HD2	1.93	0.51
3:C:375:LYS:HE2	3:C:417:TYR:OH	2.11	0.51
3:Z:551:MET:HG2	3:Z:555:GLU:CB	2.41	0.51
2:B:131:ARG:NH1	2:B:158:GLU:OE2	2.44	0.51
1:X:78:GLN:CA	1:X:78:GLN:HE21	2.22	0.51
3:Z:186:GLU:HB2	3:Z:228:SER:HB2	1.93	0.50
1:X:6:PRO:HG3	1:X:16:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:ARG:NH1	3:C:294:PRO:O	2.44	0.50
1:X:78:GLN:O	1:X:79:ILE:HG13	2.11	0.50
3:Z:455:VAL:HB	3:Z:533:THR:HB	1.93	0.50
2:B:54:ARG:NH1	2:B:102:THR:O	2.44	0.50
3:C:186:GLU:HB2	3:C:228:SER:HB2	1.93	0.50
3:C:335:SER:O	3:C:336:GLN:HB2	2.11	0.50
3:C:528:ASN:HD21	3:C:535:GLN:HG2	1.76	0.50
1:A:9:ASN:C	1:A:9:ASN:HD22	2.15	0.49
3:C:227:ASP:N	3:C:227:ASP:OD1	2.29	0.49
3:C:394:SER:HB2	3:C:445:GLY:HA3	1.94	0.49
3:Z:428:PRO:O	3:Z:429:TYR:HB2	2.12	0.49
3:Z:335:SER:HB3	3:Z:337:ARG:HG3	1.94	0.49
3:Z:227:ASP:N	3:Z:227:ASP:OD1	2.36	0.48
3:C:428:PRO:O	3:C:429:TYR:HB2	2.12	0.48
3:Z:460:GLU:CB	3:Z:462:LEU:HD13	2.43	0.48
4:L:19:DT:H2"	4:L:20:DT:O5'	2.12	0.48
2:B:59:ALA:O	2:B:143:ARG:NH2	2.41	0.48
1:X:76:ALA:HB1	1:X:79:ILE:HD11	1.96	0.48
3:C:595:ARG:HH11	4:K:17:DT:C7	2.24	0.48
1:X:58:SER:HB2	1:X:81:GLU:CD	2.34	0.48
2:Y:68:PHE:HZ	2:Y:138:SER:HB2	1.78	0.47
3:Z:451:ARG:CG	3:Z:451:ARG:NH1	2.70	0.47
1:A:78:GLN:HA	1:A:78:GLN:NE2	2.24	0.47
1:A:78:GLN:CA	1:A:78:GLN:HE21	2.23	0.47
3:C:470:TYR:CE2	3:C:584:ARG:HB3	2.49	0.47
3:Z:507:TRP:O	3:Z:515:SER:HA	2.14	0.47
3:C:299:GLU:O	3:C:316:ASP:HB2	2.14	0.47
1:X:40:SER:HB2	1:X:97:GLU:HB2	1.95	0.47
3:Z:327:LEU:HD11	3:Z:364:GLU:HG2	1.97	0.47
3:Z:292:ASP:OD1	3:Z:292:ASP:N	2.33	0.47
3:C:460:GLU:CB	3:C:462:LEU:HD13	2.45	0.47
3:Z:528:ASN:HD21	3:Z:535:GLN:HG2	1.79	0.47
3:Z:470:TYR:CE2	3:Z:584:ARG:HB3	2.50	0.47
3:C:388:PHE:HD1	3:C:448:MET:CG	2.28	0.47
1:A:15:GLN:NE2	1:X:15:GLN:HE22	2.12	0.46
1:X:1:MET:O	1:X:2:GLU:C	2.54	0.46
3:C:417:TYR:HA	3:C:421:GLY:HA3	1.97	0.46
3:Z:453:THR:OG1	3:Z:455:VAL:HG12	2.15	0.46
3:C:327:LEU:HD11	3:C:364:GLU:HG2	1.96	0.46
3:Z:303:ILE:HG12	3:Z:348:ASP:OD2	2.16	0.46
3:Z:417:TYR:HA	3:Z:421:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:CA	1:A:80:ARG:HE	2.19	0.46
3:Z:498:LYS:HD2	4:L:14:DT:H4'	1.98	0.46
1:A:40:SER:HB2	1:A:97:GLU:HB2	1.98	0.46
3:C:451:ARG:NH1	3:C:451:ARG:HG3	2.03	0.46
3:C:242:ARG:NH1	3:C:280:ASN:HA	2.31	0.45
3:Z:320:ILE:HD13	3:Z:377:VAL:HG22	1.97	0.45
3:Z:333:LYS:HB2	4:L:7:DT:OP1	2.17	0.45
3:C:320:ILE:HD13	3:C:377:VAL:HG22	1.97	0.45
3:C:488:THR:HG22	3:C:521:TYR:CE2	2.51	0.45
3:C:455:VAL:HB	3:C:533:THR:HB	1.97	0.45
3:Z:299:GLU:O	3:Z:316:ASP:HB2	2.16	0.45
3:Z:491:ALA:HB3	3:Z:516:TYR:CD2	2.52	0.45
3:C:388:PHE:HD1	3:C:448:MET:HG2	1.81	0.45
4:L:3:DT:H2"	4:L:4:DT:O5'	2.16	0.45
2:Y:132:VAL:HG22	2:Y:150:MET:HG3	1.99	0.45
1:A:78:GLN:O	1:A:79:ILE:HG13	2.17	0.45
1:A:83:THR:HB	1:A:84:THR:H	1.33	0.45
3:Z:244:TYR:HB3	3:Z:245:PRO:HD3	1.99	0.45
3:C:597:ARG:CD	4:K:17:DT:O4	2.58	0.45
3:Z:447:ASN:HB2	3:Z:450:GLU:CD	2.38	0.44
3:C:327:LEU:CD1	3:C:364:GLU:HA	2.47	0.44
3:Z:468:PRO:HB3	3:Z:586:LYS:HG2	2.00	0.44
1:A:82:PHE:CE2	2:B:156:TYR:CD1	3.06	0.44
3:C:602:ARG:HH21	3:C:604:ALA:CB	2.23	0.44
2:Y:62:PRO:O	2:Y:63:HIS:CB	2.64	0.44
3:Z:394:SER:CB	3:Z:445:GLY:HA3	2.47	0.44
1:X:78:GLN:HA	1:X:78:GLN:NE2	2.25	0.44
3:Z:263:ALA:HA	3:Z:275:GLU:CG	2.47	0.44
1:X:2:GLU:OE1	1:X:2:GLU:CA	2.66	0.44
4:L:4:DT:H2"	4:L:5:DT:H71	1.99	0.44
3:C:375:LYS:HG2	3:C:417:TYR:HE2	1.78	0.43
1:X:21:VAL:CG2	1:X:74:PHE:CZ	3.01	0.43
2:Y:125:ARG:HH11	2:Y:125:ARG:HB2	1.83	0.43
1:X:81:GLU:CD	1:X:82:PHE:N	2.72	0.43
3:C:280:ASN:HD22	3:C:280:ASN:HA	1.62	0.43
3:C:208:ARG:HH21	4:K:4:DT:P	2.41	0.43
2:Y:71:ASP:OD2	2:Y:170:HIS:CD2	2.70	0.43
1:A:81:GLU:CD	1:A:82:PHE:N	2.72	0.43
1:X:83:THR:HG22	1:X:84:THR:H	1.84	0.42
3:C:379:ALA:O	3:C:401:MET:HA	2.19	0.42
3:C:595:ARG:HD2	4:K:17:DT:H72	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:5:THR:HG22	1:X:22:ARG:HB2	2.00	0.42
3:Z:327:LEU:CD1	3:Z:364:GLU:HA	2.49	0.42
2:B:131:ARG:HG2	2:B:131:ARG:NH1	2.31	0.42
3:C:514:ARG:HG2	3:C:515:SER:N	2.27	0.42
4:K:4:DT:C2'	4:K:5:DT:H71	2.49	0.42
4:L:3:DT:O2	4:L:4:DT:H71	2.20	0.42
2:Y:80:PHE:HA	2:Y:162:HIS:CE1	2.53	0.42
3:Z:525:LEU:O	3:Z:539:SER:HA	2.19	0.42
1:X:82:PHE:HB2	1:X:83:THR:H	1.54	0.42
3:C:327:LEU:HD12	3:C:364:GLU:HA	2.02	0.42
2:B:94:VAL:HG23	2:B:111:LEU:HD21	2.01	0.42
3:Z:263:ALA:HA	3:Z:275:GLU:CD	2.40	0.42
3:C:263:ALA:HA	3:C:275:GLU:CD	2.40	0.42
3:C:457:VAL:HA	3:C:462:LEU:HD22	2.02	0.42
3:Z:352:ARG:NH2	3:Z:429:TYR:HA	2.32	0.42
3:C:244:TYR:HB3	3:C:245:PRO:HD3	2.02	0.42
3:Z:389:GLY:HA2	3:Z:431:ASN:H	1.85	0.42
1:A:81:GLU:C	1:A:82:PHE:CD2	2.92	0.42
2:Y:94:VAL:HG23	2:Y:111:LEU:HD21	2.01	0.42
3:Z:233:ALA:HA	3:Z:276:ILE:O	2.19	0.41
3:C:357:THR:OG1	3:C:444:ALA:HB3	2.19	0.41
3:Z:384:LYS:HE3	3:Z:445:GLY:O	2.20	0.41
2:B:61:GLN:C	2:B:63:HIS:N	2.72	0.41
1:A:41:ASP:O	1:A:42:LEU:HB2	2.20	0.41
2:B:81:VAL:HA	2:B:130:VAL:O	2.20	0.41
1:X:84:THR:HG22	1:X:85:VAL:H	1.85	0.41
3:Z:607:ASP:OD1	3:Z:607:ASP:C	2.59	0.41
3:Z:587:MET:CE	3:Z:594:ALA:HB1	2.51	0.41
1:X:6:PRO:HB2	1:X:8:ILE:CG2	2.51	0.41
3:Z:366:PHE:HB3	3:Z:367:PRO:HD3	2.03	0.41
1:A:21:VAL:CG2	1:A:74:PHE:CZ	3.01	0.41
1:A:95:LEU:HD12	1:A:95:LEU:O	2.20	0.41
3:C:263:ALA:HA	3:C:275:GLU:CG	2.51	0.41
4:K:4:DT:H2"	4:K:5:DT:H71	2.03	0.41
2:B:131:ARG:CG	2:B:131:ARG:HH11	2.32	0.40
3:C:322:ASP:HA	3:C:375:LYS:HE3	2.03	0.40
4:L:13:DT:H2'	4:L:14:DT:H72	2.04	0.40
1:X:83:THR:HG23	1:X:90:ASP:HA	2.03	0.40
2:B:154:ILE:HD12	3:C:608:PHE:HE1	1.86	0.40
3:C:380:PHE:HB3	3:C:383:VAL:HG21	2.04	0.40
2:Y:136:LEU:O	2:Y:137:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	104/114 (91%)	92 (88%)	10 (10%)	2 (2%)	8 26
1	X	104/114 (91%)	93 (89%)	9 (9%)	2 (2%)	8 26
2	B	118/136 (87%)	111 (94%)	3 (2%)	4 (3%)	3 13
2	Y	118/136 (87%)	111 (94%)	6 (5%)	1 (1%)	19 49
3	C	429/444 (97%)	399 (93%)	21 (5%)	9 (2%)	7 23
3	Z	429/444 (97%)	398 (93%)	25 (6%)	6 (1%)	11 34
All	All	1302/1388 (94%)	1204 (92%)	74 (6%)	24 (2%)	8 28

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	THR
2	B	63	HIS
2	B	65	ASP
3	C	216	GLU
3	C	336	GLN
3	C	449	ALA
3	Z	449	ALA
3	C	448	MET
1	X	2	GLU
3	C	212	ASN
3	Z	514	ARG
2	B	62	PRO
2	B	64	PRO
3	C	237	ASN
3	C	429	TYR
3	C	591	ASN
1	X	82	PHE

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Mol	Chain	Res	Type
3	Z	420	ASP
3	Z	429	TYR
3	Z	593	THR
3	C	420	ASP
2	Y	63	HIS
3	Z	237	ASN
1	A	71	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	96/101 (95%)	81 (84%)	15 (16%)	2 8
1	X	96/101 (95%)	78 (81%)	18 (19%)	1 5
2	B	107/118 (91%)	96 (90%)	11 (10%)	7 21
2	Y	107/118 (91%)	93 (87%)	14 (13%)	4 12
3	C	370/374 (99%)	340 (92%)	30 (8%)	11 33
3	Z	370/374 (99%)	342 (92%)	28 (8%)	13 36
All	All	1146/1186 (97%)	1030 (90%)	116 (10%)	7 22

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	9	ASN
1	A	47	ILE
1	A	52	ASP
1	A	59	THR
1	A	66	LYS
1	A	69	ASP
1	A	74	PHE
1	A	78	GLN
1	A	80	ARG
1	A	83	THR

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Mol	Chain	Res	Type
1	A	84	THR
1	A	93	LEU
1	A	109	LEU
1	A	111	SER
2	B	63	HIS
2	B	74	GLU
2	B	104	GLN
2	B	106	GLU
2	B	107	VAL
2	B	123	GLU
2	B	125	ARG
2	B	131	ARG
2	B	173	VAL
2	B	174	THR
2	B	175	ARG
3	C	198	LYS
3	C	200	ARG
3	C	213	GLN
3	C	227	ASP
3	C	249	GLU
3	C	288	THR
3	C	292	ASP
3	C	315	CYS
3	C	330	ILE
3	C	362	THR
3	C	372	VAL
3	C	381	LYS
3	C	398	SER
3	C	400	THR
3	C	401	MET
3	C	406	ASP
3	C	407	ILE
3	C	414	ARG
3	C	429	TYR
3	C	451	ARG
3	C	483	GLU
3	C	485	LEU
3	C	520	GLU
3	C	526	SER
3	C	535	GLN
3	C	556	LEU
3	C	586	LYS

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Mol	Chain	Res	Type
3	C	589	THR
3	C	593	THR
3	C	610	LYS
1	X	1	MET
1	X	2	GLU
1	X	6	PRO
1	X	9	ASN
1	X	39	THR
1	X	47	ILE
1	X	59	THR
1	X	66	LYS
1	X	69	ASP
1	X	73	SER
1	X	74	PHE
1	X	78	GLN
1	X	80	ARG
1	X	82	PHE
1	X	83	THR
1	X	84	THR
1	X	90	ASP
1	X	93	LEU
2	Y	65	ASP
2	Y	74	GLU
2	Y	98	VAL
2	Y	104	GLN
2	Y	106	GLU
2	Y	107	VAL
2	Y	123	GLU
2	Y	125	ARG
2	Y	140	GLN
2	Y	145	ILE
2	Y	146	SER
2	Y	173	VAL
2	Y	174	THR
2	Y	175	ARG
3	Z	198	LYS
3	Z	200	ARG
3	Z	213	GLN
3	Z	227	ASP
3	Z	249	GLU
3	Z	288	THR
3	Z	291	THR

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Mol	Chain	Res	Type
3	Z	292	ASP
3	Z	315	CYS
3	Z	328	SER
3	Z	330	ILE
3	Z	339	VAL
3	Z	372	VAL
3	Z	381	LYS
3	Z	400	THR
3	Z	401	MET
3	Z	406	ASP
3	Z	407	ILE
3	Z	414	ARG
3	Z	429	TYR
3	Z	451	ARG
3	Z	483	GLU
3	Z	485	LEU
3	Z	520	GLU
3	Z	535	GLN
3	Z	556	LEU
3	Z	586	LYS
3	Z	610	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	15	GLN
1	A	44	ASN
1	A	78	GLN
2	B	90	ASN
2	B	93	ASN
2	B	104	GLN
2	B	109	GLN
2	B	149	HIS
2	B	170	HIS
3	C	261	ASN
3	C	280	ASN
3	C	369	ASN
3	C	528	ASN
3	C	535	GLN
3	C	542	ASN
3	C	557	HIS

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Mol	Chain	Res	Type
1	X	9	ASN
1	X	44	ASN
1	X	78	GLN
2	Y	61	GLN
2	Y	77	GLN
2	Y	104	GLN
2	Y	109	GLN
2	Y	149	HIS
2	Y	170	HIS
3	Z	261	ASN
3	Z	280	ASN
3	Z	369	ASN
3	Z	423	HIS
3	Z	500	ASN
3	Z	528	ASN
3	Z	542	ASN
3	Z	557	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	108/114 (94%)	-0.10	3 (2%)	53	43	28, 47, 87, 108	0
1	X	108/114 (94%)	0.02	5 (4%)	32	22	28, 54, 94, 125	0
2	B	122/136 (89%)	-0.23	2 (1%)	72	66	22, 45, 96, 120	0
2	Y	122/136 (89%)	-0.27	3 (2%)	57	47	24, 46, 87, 120	0
3	C	433/444 (97%)	0.06	21 (4%)	30	21	28, 68, 121, 150	0
3	Z	433/444 (97%)	0.07	28 (6%)	18	11	26, 67, 122, 172	0
4	K	25/62 (40%)	1.14	5 (20%)	1	0	65, 119, 165, 194	0
4	L	20/62 (32%)	0.69	2 (10%)	7	4	79, 128, 166, 180	0
All	All	1371/1512 (90%)	0.02	69 (5%)	28	19	22, 62, 121, 194	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	441	GLY	9.8
1	X	85	VAL	7.6
1	A	85	VAL	6.4
3	Z	448	MET	5.8
3	Z	388	PHE	5.4
4	K	10	DT	5.4
2	B	112	ASP	5.3
3	Z	591	ASN	5.1
2	Y	112	ASP	4.7
3	Z	441	GLY	4.7
3	C	214	ARG	4.4
3	Z	589	THR	4.3
3	Z	588	ASP	4.3
3	Z	590	PHE	4.0
3	Z	466	GLU	4.0
3	C	216	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
2	Y	140	GLN	3.9
4	K	22	DT	3.9
3	C	590	PHE	3.8
3	C	419	ASN	3.6
1	X	54	ASP	3.6
1	X	84	THR	3.6
3	C	442	GLY	3.6
3	C	290	ALA	3.6
1	X	1	MET	3.6
3	Z	593	THR	3.5
3	C	425	GLN	3.4
4	K	11	DT	3.3
3	C	423	HIS	3.2
3	Z	449	ALA	3.1
3	Z	446	ALA	3.1
3	Z	594	ALA	3.1
3	Z	587	MET	2.9
3	C	331	VAL	2.9
3	C	591	ASN	2.8
3	Z	447	ASN	2.8
3	Z	592	ASP	2.7
3	Z	595	ARG	2.7
3	C	211	SER	2.6
3	Z	314	GLN	2.6
1	A	84	THR	2.6
3	C	431	ASN	2.5
2	B	139	PHE	2.5
3	C	213	GLN	2.5
3	Z	279	GLU	2.5
3	C	337	ARG	2.4
3	Z	468	PRO	2.4
4	K	21	DT	2.3
3	Z	289	ASP	2.3
2	Y	139	PHE	2.3
3	C	589	THR	2.3
3	Z	565	SER	2.2
4	K	24	DT	2.2
3	Z	425	GLN	2.2
3	Z	422	ALA	2.2
3	Z	390	GLY	2.2
4	L	20	DT	2.2
4	L	21	DT	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	70	ALA	2.2
3	C	420	ASP	2.1
3	Z	431	ASN	2.1
3	C	465	SER	2.1
3	Z	566	GLU	2.1
1	A	71	GLY	2.1
3	C	215	GLY	2.1
3	C	467	LYS	2.1
3	Z	427	GLN	2.1
3	Z	214	ARG	2.0
3	C	402	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	Z	701	1/1	0.98	0.07	68,68,68,68	0
5	ZN	C	701	1/1	0.99	0.05	72,72,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.